Mastering models

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Computer-Assisted Structure Elucidation. By Neil A. B. Gray. *Wiley:1986. Pp.536. $54.95, £52.70.*

MANY chemists enjoy the intellectual challenge of structure elucidation. To others, however, the process is merely a prelude to synthetic, mechanistic or biochemical studies, so short cuts to the structure are warmly welcomed. The most important short cuts, other than X-ray crystallography, are the spectroscopic methods: IR, NMR, UV and mass spectra all give detailed information about different aspects of molecular structure, but generally do not lead directly to a complete structure. The chemist therefore has to create a set of hypothetical structures and then test their predicted properties against the experimental evidence. The structures that fail are discarded, while those that pass are subjected to further tests. With luck, one is left with a unique correct structure. Sometimes, several candidates fit all the evidence and additional experiments are necessary; on other occasions all the structures the chemist can think of must be discarded — we tend only to propose structure types that are familiar or precedented, while nature is more creative and less prejudiced.

In this book, Neil Gray has attempted to show how computers can help in all phases of the structure-elucidation process. He explains clearly, and with abundant chemical examples, the principles behind pattern recognition, spectrum matching, and the generation and testing of structures. The book is derived from Gray's association with Djerassi's historic DENDRAL project of the 1970s, and in places it perhaps gives undue emphasis to the details of that particular project — for example, the algorithms for generating and checking all possible structures with a particular formula are described in more detail than most chemists need. The reference lists are comprehensive, and also cover topics such as spectroscopic data bases and synthesis-analysis programs. Unfortunately the literature coverage peters out in early 1983, so there is no mention of automated analysis (using pattern recognition algorithms) of COSY NMR spectra or of NOE data.

Gray is careful to emphasize both the strengths of the computer, as in the generation of possible structures, and its weaknesses, as in the matching of spectroscopic data to unusual structural features. We all know that the computer is indispensable for collecting and processing spectroscopic data; Gray shows us that we should also use it for generating structures as candidates in the elucidation process, because that is a mechanical job the machine does better than we do. However, it is clear that, as yet, we do not know how to program the subtle interpretation of information or the inspirational leap to the right answer, presumably because we don't know how we ourselves do it.

This, then, is an interesting book which will be useful for chemists who want to know about computers or computer scientists who want to know about chemistry. It also challenges us to ponder upon, and admire, the way that the human mind goes about the business of solving problems. □

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